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Short note on the bending models for a membrane in capsule mechanics: Comparison between continuum and discrete models

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ABSTRACT

With regard to the out-of-plane bending energy of an elastic surface membrane, capsule deformation was compared between Helfrich's isotropic continuum model and discrete models using a triangulated surface. The in-plane deformation of the membrane was modeled by the neo-Hookean or Skalak law. Two mechanical problems were numerically simulated. One was the deformation of a spherical capsule under simple shear flow and the other was the equilibrium shape of a capsule with a nonzero excess surface area, assuming the shape mechanics of a normal red blood cell. The numerical simulations demonstrated that a discrete model based on locally averaged mean curvature satisfactorily reproduces the mechanical behavior determined by Helfrich's isotropic continuum model, whereas a discrete model without the averaging exhibited different deformation behavior. Differences in the mechanical behavior between bending models may cause differences in estimated bending rigidity values of up to one order of magnitude.

1. Introduction

A capsule is defined as a fluid drop encapsulated by a surface membrane, and such structures are observed in vesicles and red blood cells. The surface membrane exhibits rich deformation behavior depending on external forces, and its mechanics are broadly divided into in-plane and out-of-plane deformation. In-plane deformation may be modeled by a Newtonian interface [1], a neo-Hookean membrane [2], and a red blood cell membrane [3]. An out-of-plane bending deformation model is mostly based on curvature elasticity [4–6]. Numerical simulations using these membrane models are important for understanding capsule mechanics, where triangular discretization can replicate complicated membrane geometries and mechanics [7–20].

This note focuses on the out-of-plane bending deformation models using a triangulated surface membrane. In the well-known isotropic continuum model of Helfrich [5], the elastic free energy W_B of a closed membrane surface A is described as

$$W_B = \frac{1}{2} B \int_A (2H - C_0)^2 dA, \tag{1}$$

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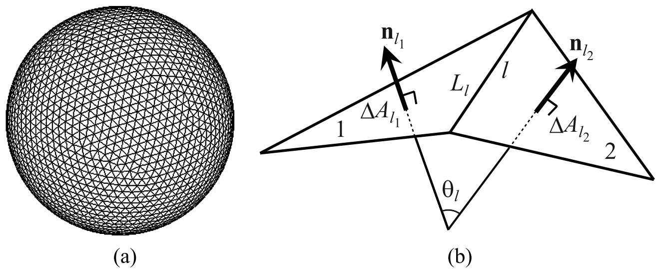

Fig. 1. Numerical model of capsule mechanics: (a) surface membrane is discretized by triangular elements and (b) two triangular elements 1 and 2 neighbor each other along edge l with length L_l and angle θ_l. The outer normal vectors $\boldsymbol{n}_{l_1}$ and $\boldsymbol{n}_{l_2}$ and the surface area ΔA_{l_1} and ΔA_{l_2} of the two elements are also illustrated.

where $H = \frac{1}{2}(C_1 + C_2)$ is the spontaneous mean curvature, which may be determined by the two principal curvatures C_1 and C_2 ($C_1 \geq C_2$), C_0 is the reference curvature, and B is the bending rigidity. To compute the membrane force density for simulating the deformation of a capsule under simple shear flow, Pozrikidis [9] used the equivalent local constitutive equation that relates the bending moment to the curvature. Alternatively, Yazdani and Bagchi [16,17] and Boedec et al. [20] adopted the force density equation derived from Eq. (1) [21]. These methods essentially provide the same membrane force density.

On the other hand, the discrete model by Kantor and Nelson [22] utilized the potential energy as an increasing function of the angle between two neighboring triangular elements. Subsequently, Jülicher [23] and Gompper and Kroll [24] modified the discrete model by considering the local average of the mean curvature. Discrete models have been used as an alternative to Eq. (1) [10–12,18,25–28]. However, the differences in the mechanical behavior described by continuum and discrete models have not yet been clarified by direct numerical simulations. This is important when capsule deformation is small because the out-of-plane bending deformation of the membrane governs capsule mechanics, whereas the importance of out-of-plane bending decays as the deformation increases up to the point at which capsule deformation is mostly controlled by in-plane deformation characteristics [18,29].

In this study, capsule deformation was numerically simulated for two cases. First, the deformation of a spherical capsule under simple shear flow, a well-known problem in capsule mechanics [30,31]. Second, the equilibrium shape of a capsule with a nonzero excess surface area obtained by relaxation toward equilibrium in the absence of an imposed flow, which assumes the shape mechanics of a normal red blood cell [32]. By comparing simulated capsule deformations, it is demonstrated that the discrete model based on the local average of the mean curvature [23] satisfactorily reproduces the capsule deformation by Helfrich's model, whereas discrete models without the averaging exhibit different deformation behavior.

2. Methods

2.1. Capsule mechanics model

The surface of the capsule is divided into triangular elements, as shown in Fig. 1(a). The membrane generates an elastic force against the in-plane deformation as well as the out-of-plane bending deformation. The in-plane deformation is modeled by the neo-Hookean law [2]

$$T_1 = \frac{G}{\lambda_1 \lambda_2}\left[\lambda_1^2 - \frac{1}{\lambda_1^2 \lambda_2^2}\right], \tag{2}$$

or the Skalak law proposed for a red blood cell [33,34]

$$T_1 = G\frac{\lambda_1}{\lambda_2}\left[\left(\lambda_1^2 - 1\right) + C_A \lambda_2^2\left(\lambda_1^2 \lambda_2^2 - 1\right)\right] \tag{3}$$

Here, T_1 is the principal tension, λ_1 and λ_2 ($\lambda_1 \geq \lambda_2$) are the principal stretches, and G is the shear modulus. In Eq. (3), C_A is an elastic constant that determines the area dilation modulus $G(1 + 2C_A)$. The other principal tension T_2 ($T_1 \geq T_2$) is obtained by reversing indices 1 and 2. In Section 2.4, the neo-Hookean law (Eq. (2)) is used for the deformation of a spherical capsule under shear flow in accordance with published numerical studies [8,9,13]. Because the Skalak law (Eq. (3)) expresses the in-plane elasticity of a red blood cell membrane effectively [34], it is used to determine the equilibrium shape of a capsule with an excess surface area that assumes the shape mechanics of a red blood cell. Helfrich's model (Eq. (1)) is considered for the out-of-plane bending deformation. The details are described in Section 2.2.

A constraint of constant total volume may be imposed on the capsule [18,27,35]. The elastic energy Γ_V owing to a deviation in volume V from the reference V_0 is described using the bulk modulus k_V as

$$\Gamma_V = \frac{k_V}{2}\left(\frac{V - V_0}{V_0}\right)^2 V_0. \tag{4}$$